COMETARY COMA IONS

A. C. AIKIN

APRIL 1974

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For information concerning availability of this document contact:

Technical Information Division, Code 250 Goddard Space Flight Center Greenbelt, Maryland 20771

(Telephone 301-982-4488)

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by

A. C. Aikin
Laboratory for Planetary Atmospheres
NASA Goddard Space Flight Center
Greenbelt, Maryland

Abstract

For comets whose nuclei are composed of water ice conglomerates it is shown that the ion H_3O^+ can predominate to distances of 5000 km in the subsolar direction. Beyond this distance H_2O^+ is the most important ion. The crossover point is a sensitive function of the rate of evaporation from the nucleus. The presence of ammonia or metals such as sodium, in concentrations greater than 0.1% H_2O , can lead to NH_4^+ and Na^+ ions.

Observations of hydrogen Lyman alpha emission from comets (Bertaux and Blamont, 1970; Code and Savage, 1972), have substantiated the suggestion that water is the major constituent of many cometary comas. The presence of water also explains the observation of OH radicals and ions as well as the identification of $\rm H_2O^+$ in comet tails (Herzberg and Lew, 1974). Under these circumstances recent models show that the inner coma (distances less than 10,000 km from the nucleus) is composed principally of $\rm H_2O$ with a small amount of OH, H and O resulting from photodissociation (Mendis et al., 1972). It is the purpose of this note to discuss the ions which can occur in the coma when water is the major constituent.

The inner coma can be described as consisting principally of undissociated H_2O , whose density as a function of radial distance, r, from the nucleus is described by the relationship

$$\rho_{\mathbf{r}} = \rho_{0}(\frac{\mathbf{r}_{0}}{\mathbf{r}})^{2}$$

where ρ_0 and r_0 are the density and distance at some reference point and ρ_r is the density at r. Values of ρ_0 and r_0 are assumed for the model and can be typically 2.5x10¹² cm³ and 10 km (Ip and Mendis, 1973). The ionization rate of water, I, by solar radiation of wavelength $\lambda < 984$ Å is

$$I(\lambda) = \sigma(\lambda)\phi(\lambda)(\frac{1}{R})^2 e^{-\tau(r,\lambda)} sec^{-1}$$

where R is the cometary heliocentric distance and τ is the optical depth given by $\tau(r,\lambda) = \sigma(\lambda) \rho_r r$ at the subsolar point. At a distance of lAU the value of I_{∞} is 5 x 10⁻⁷ sec⁻¹. The ionization production function for H_2O^+ ions is given by

$$q = \frac{n(H_2O)_0}{r^2} (r_0^2) I(\lambda)$$

Assuming that $\rho_0 = 2.5 \times 10^{12} \text{ cm}^{-3}$ a maximum q of 2 x 10^2 occurs at the value of r where $\tau = 2$.

The ions ${\rm H_2O}^+$ can be lost by several processes including photo-dissociation ${\rm J_{H_2O}}^+$, dissociative electron-ion recombination $\alpha_{\rm H_2O}^+$, and ion-molecule reactions, ${\rm k_i}$. The relative importance of these processes can be seen by comparing typical time constants for each. The photodissociation rate of ${\rm H_2O}^+$ is probably comparable to that for ${\rm H_2O}$ which has a value of 2 x ${\rm 10^5}$ seconds (Jackson, 1972). Maximum electron densities are ${\rm 10^5}$ cm⁻³ and $\alpha_{\rm H_2O}^+$ can be ${\rm 10^{-6}}$ cm³ sec⁻¹ so that τ_{α} = 10 seconds. If ${\rm k_1}$ = ${\rm 10^{-10}}$ cm³ sec⁻¹ and ${\rm n(H_2O)}$ = ${\rm 10^{11}}$ cm⁻³, $\tau_{\rm k}$ = ${\rm 10^{-1}}$ seconds. One may conclude that photodissociation is negligible in comparison with dissociative recombination and ion-molecule reactions for the loss of ${\rm H_2O}^+$.

Reactions of possible importance to a water ice comet are

$$H_2O^+ + H_2O \rightarrow H_3O^+ + OH$$
 $k_1 = 4.9 \times 10^{-10} \text{ cm}^3 \text{ sec}^{-1}$

and

$$H_2O^+ + H_2 \rightarrow H_3O^+ + H$$
 $k_2 = 1.4 \times 10^{-9} \text{ cm}^3 \text{ sec}^{-1}$

The rate coefficient k_1 and k_2 have been measured in the laboratory by Thynne and Harrison (1966) and Fehsenfeld et al. (1967). Since the ratio $H_2O/H_2 \gg 1$, the first of these is the most significant. Both processes lead to the formation of hydronium H_3O^+ . The radical OH^+ will react in a similar manner through the processes

$$OH^{+} + H_{2} \rightarrow H_{2}O^{+} + H$$
 $k_{3} = 1.5 \times 10^{-9} \text{ cm}^{3} \text{ sec}^{-1}$ and

$$OH^{+} + H_{2}O \rightarrow H_{3}O^{+} + O \quad k_{4} = 1.4 \times 10^{-9} \text{ cm}^{3} \text{ sec}^{-1}$$

The steady-state conservation equations governing ions produced in a pure H₂O system can be written as

$$\frac{1}{r^2} \frac{dV_e r^2 n_e}{dr} = q - \alpha n_e^2$$

$$\frac{1}{r^2} \frac{dv_{\text{H}_20} + r^2 [\text{H}_20]^+}{dr} = q - \alpha n_e [\text{H}_20]^+ - k_1 [\text{H}_20] [\text{H}_20]^+$$

$$\frac{1}{r^2} \frac{dV_{H_30} + r^2[H_30]^+}{dr} = k_1[H_20][H_20]^+ - \alpha n_e[H_30]^+$$

If it is assumed that the dissociative recombination coefficient for all species of ion is 10^{-6} cm³ sec⁻¹ and that the velocity of all species is constant at 1 km/sec, then Figure 1 summarizes the resulting solution of the continuity equations. In this analysis

$$n_e = [H_20]^+ + [H_30]^+$$

all other species of ion being neglected.

For distances less than 5000 km $\rm H_30^+$ is the principle ion. Beyond this distance $\rm H_20^+$ becomes dominant and can be swept into the tail if not dissociated. The total electron density varies slightly more than an order of magnitude between $\rm 10^2$ and $\rm 10^4$ km. The spectrum of the ion $\rm H_30^+$ is unknown. Important energy level transitions are not available. Such transitions should be defined and a search made for $\rm H_30^+$ near the cometary nucleus.

It should be noted that ${\rm H_3O}^+$ can be lost by charge exchange with neutral metals as for example

$$H_3O^+ + Na \rightarrow Na^+ + H_3O$$

However, in order to be important the metal atom density must exceed $10^7~{\rm cm}^{-3}$ in the inner comma. Similar concentration of ammonia will cause a loss of ${\rm H_3O^+}$ thru the proton transfer reaction.

$$H_30^+ + NH_3 \rightarrow NH_4^+ + H_20$$

It has been shown that although $\mathrm{H_2O^+}$ is the ion initially formed in the inner coma, $\mathrm{H_3O^+}$ will be the principal ion to distances from the comet nucleus of several thousand kilometers. Beyond this $\mathrm{H_2O^+}$ is the principal ion if undissociated. Sufficient quantities of ammonia and metals such as sodium will lead to $\mathrm{NH_h}^+$ and $\mathrm{Na^+}$ within the coma.

Since the ion composition is a sensitive function of the water evaporation rate from the nucleus, measurements of coma ions will provide important information on the behavior of the cometary nucleus as well as the coma.

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Figure 1: The distribution of electron density N_e , and the ions ${\rm H_30}^+$ and ${\rm H_20}^+$ as a function of distance from the nucleus in the subsolar direction.

